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A COMPARISON BETWEEN THE TOTAL LAGRANGIAN SCHEME (TLS) AND THE PREDOMINAT TWIN REORIENTATION (PTR) METHODS TO ANALYZE THE TWINNING DEFORMATIONS IN A RATE DEPENDENT CRYSTAL PLASTICITY MODEL

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Abstract. Materials with Hexagonal-Closed Pack (HCP) crystal structures, as for example the magnesium and titanium alloys, have a small number of active slip systems at room temperature. This fact makes twinning as a predominant deformation mechanism and thus essential for the accurate prediction of plastic deformations and texture evolution. Also, because of the directional property of the twinning mechanism, different responses are obtained for tension and compression, explaining the asymmetric behaviour of HCP metals. As reported by Van Houtte [1], the twinning mechanism is also important for low stacking fault energy Face Centred Cubic (FCC) metals.

In this work, we developed two types of a finite element analysis code, based on the crystal plasticity theory, including twinning as a dominant deformation mechanism. The first twinning model is based on the Predominat Twin Reorientation (PTR) scheme, suggested initially by Van Houtte [1], and the second one is based on the Total Lagragian Scheme (TLS), suggested by Kalidindi [2]. The PTR model has the advantage of being simple and computationally efficient. On the other hand, the TLS model has some advantages when compared with the PTR model that are: i) the possibility of continuously consider the texture's evolution from both slip and twinning deformations; ii) the consideration of slip in the twinned regions.

In the present paper, the two models are compared for a tension and a compression simulation for a FCC material.

1 INTRODUCTION

Materials with Hexagonal-Closed Packed (HCP) crystal structures, as for example the magnesium and titanium alloys, have a small number of active slip systems at room temperature. This fact makes twinning a predominant deformation mechanism, essential for the accurate prediction of plastic deformations and texture evolution. Also, because of the directional property of the twinning mechanism, different responses are obtained for tension and compression, explaining in this way the asymmetric behaviour of HCP materials. As reported by Van Houtte [1], the twinning mechanism is also important for low stacking fault energy Face Centred Cubic (FCC) metals.

To predict the elasto-plastic behaviour of HCP materials, several material models were suggested in the last years. As an example, the Predominant Twin Reorientation (PTR) method was initially proposed by van Houtte [1]. This innovative model evaluates the twinning deformation from the crystal plasticity theory. After reaching a threshold value for the twinning volume fraction, the deformation by twinning causes reorientation of the grains almost instantaneously. This is in contrast with the TLS method that considers twinning reorientation continuously.

To treat both slip, twinning and slip in the twined regions, Kalidindi[2] suggested the Total Lagragian Scheme (TLS). This work is based on the decomposition of the deformation gradient into components related with slip, twinning and slip deformations in the twined regions. The set of nonlinear constitutive equations for slip, twinning and slip-twinning deformation modes are fully linearized for a single Crystal. In this way, a fully implicit time integration schemes can be obtained.

2 KINEMATICS AND CONSTITUTIVE RELATIONS

2.1 Total Lagragian Scheme (TLS)

To consider twinning and slip deformations in the twined area, the decomposition of the velocity gradient tensor should be defined as follows,

$$\mathbf{L}^p = \left(1 - \int \sum_{\beta} \dot{f}^{(\beta)} dt\right) \sum_{\alpha} \dot{\gamma}_s^{(\alpha)} \left(\mathbf{s}_s^{(\alpha)} \otimes \mathbf{m}_s^{(\alpha)}\right) + \sum_{\beta} \dot{f}^{(\beta)} \gamma_{twc}^{(\beta)} \left(\mathbf{s}_t^{(\beta)} \otimes \mathbf{m}_t^{(\beta)}\right) + \sum_{\beta} \int \dot{f}^{(\beta)} dt \sum_{\alpha} \dot{\gamma}_{st}^{(\alpha,\beta)} \left(\mathbf{s}_{st}^{(\alpha,\beta)} \otimes \mathbf{m}_{st}^{(\alpha,\beta)}\right) \tag{1}$$

where,

$\mathbf{L}^p$: plastic velocity gradient

$\dot{f}^{(\beta)}$: rate of the volume fraction of the β twin system

$\dot{\gamma}_s^{(\alpha)}$: Slip rate of α slip system

$\mathbf{s}_s^{(\alpha)}, \mathbf{m}_s^{(\alpha)}$: Normalized vector of slip direction and normal to slip plane of α slip system

$\gamma_{twc}^{(\beta)}$: Characteristic shear strain of β twinning system

$\mathbf{s}_t^{(\beta)}, \mathbf{m}_t^{(\beta)}$: Normalized vector of twinning direction and normal to twinning plane of β twinning system

$\dot{\gamma}_{st}^{(\alpha,\beta)}$: Slip rate of α slip system in β twinning system

$\mathbf{s}_{st}^{(\alpha,\beta)}, \mathbf{m}_{st}^{(\alpha,\beta)}$: Normalized vector of slip direction and normal to slip plane of α slip system in β twined area

The first term on the right hand side of eq. (1) means pure slip deformation in the non-twined area. The second term means twinning deformation and the last term means slip deformation in the twined area (Fig.1). The shear slip rate and the volume fraction rate are obtained from the Pan-Rice formula as follows,

$$\dot{\gamma}_s^{(\alpha)} = \dot{\gamma}_0 \,\mathrm{sgn}\left(\tau_s^{(\alpha)}\right)\left|\frac{\tau_s^{(\alpha)}}{g_s^{(\alpha)}}\right|^{\frac{1}{m}} \quad , \quad \dot{f}^{(\beta)} = \frac{\dot{f}_0}{\gamma_{twc}^{(\beta)}}\left(\frac{\tau_t^{(\beta)}}{g_t^{(\beta)}}\right)^{\frac{1}{m}} \tag{2}$$

where $\tau, g, \dot{\gamma}_0, \dot{f}_0$ and m are the resolved shear stress, the critical resolved shear stress, the reference shear slip rate, the reference twinning rate and the rate sensitivity coefficient, respectively. Because of the asymmetry or polarity of the twinning mechanism, the following constraints should be applied,

$$\dot{f}^{(\beta)} = 0 \quad if\ \tau_t^{(\beta)} \leq 0\ or \int \sum_{\beta} \dot{f}^{(\beta)} dt \geq f^{threshold} \tag{3}$$

The threshold value for the TLS model means that twinning is finished after the accumulated volume fraction overcomes this value. These constraints for twinning are validated experimental and they explain the asymmetrical stress behavior between tension and compression deformation modes.

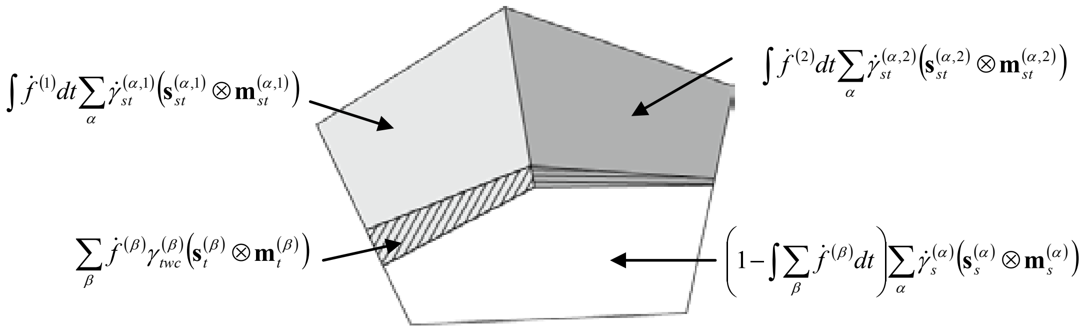

Figure 1: Schematic illustration of decomposition of velocity gradient

In order to obtain the slip shear strain rate at each slip system and the rate of volume fraction for twinning, the rate dependent crystal plasticity approach of Yoon et al. [3] is considered in this work. According to Yoon et al. [3], the Jaumann rate of Kirchhoff stress is defined as,

$$\overset{\nabla\, kirch}{\tau} = \mathbf{C} : \mathbf{D} - \sum_{\alpha} (1 - f) \dot{\gamma}_s^{(\alpha)} \mathbf{R}_s^{(\alpha)} - \sum_{\beta} \dot{f}^{(\beta)} \gamma_{twc}^{(\beta)} \mathbf{R}_t^{(\beta)} - \sum_{\beta} f^{(\beta)} \sum_{\alpha} \dot{\gamma}_{st}^{(\alpha,\beta)} \mathbf{R}_{st}^{(\alpha,\beta)} \tag{4}$$

As can be seen from equation (4), the Jaumann rate of Kirchhoff stress includes contributions from slip, twin and slip deformations in the twinned regions allowing in this way a more accurate prediction for metals with dominant twinning deformation mechanisms.

2.2 Predominat Twin Reorientation (PTR) method

In the Total Lagragian Scheme, the number of deformation systems is very high and, as a result, the CPU cost increases considerably. The PTR model doesn't include slip deformations in the twinned areas. Also, the twinning mechanisms are only effective after a threshold value for the twinning volume fraction is achieved. These facts make the Predominat Twin Reorientation method computationally more effective than TLS method.

In the Predominat Twin Reorientation method, the velocity gradient is decomposed as follows,

$$\mathbf{L}^p = \sum_{\alpha} \dot{\gamma}_s^{(\alpha)} \left(\mathbf{s}_s^{(\alpha)} \otimes \mathbf{m}_s^{(\alpha)} \right) + \sum_{\beta} \dot{f}^{(\beta)} \gamma_{twc}^{(\beta)} \left(\mathbf{s}_t^{(\beta)} \otimes \mathbf{m}_t^{(\beta)} \right) \tag{5}$$

which means that only the deformation by slip and twinning are included in the velocity gradient. In the PTR method, the accumulated volume fraction for twinning is tracked carefully. However, before the accumulated volume fraction reaches a threshold value, the grain is reoriented only by slip deformations. The threshold value is a parameter that can be fitted experimentally. According to Choi et al. [4], this threshold value can be defined as

$$f^{threshold} = C_{th1} + C_{th2} f^{accumulated} \tag{6}$$

where Cth1 and Cth2 are material constants. The accumulated twined volume fractions from all of the twinning systems are compared with this threshold value at each time step. After the accumulated volume fraction reaches the threshold value, the grain is reoriented with respect to the dominant twinning deformation system.

3 RESULTS AND DISCUSSION

3.1 Analysis conditons

We have developed an analysis code based on both PTR and TLS methods for ABAQUS/Standard 6.10-1 user material routine (UMAT). Table 1 shows the material parameters used in the analysis. In the simulations, we used the same material parameters for both slip and twinning deformations. Also, we employed 12 slip systems, {111}<110>, and 12 twinning systems, {111}<112>, for a FCC material. We implemented the hardening rule for both slip and twinning systems described in the below equation,

$$\begin{gathered} g = H_1 \left(H_2 + \sum_{\alpha} \left| \gamma^{(\alpha)} \right| dt \right)^{H_3} \\ \Delta g^{(\alpha)} = \frac{\partial g}{\partial \dot{\gamma}^{(\alpha)}} \sum_{\phi} H_{\alpha\phi} \left| \dot{\gamma}^{(\alpha)} \right| \end{gathered} \tag{7}$$

For the TLS model, the threshold value for the twined volume fraction was set to 0.8. For the PTR model, we set the same material parameters Cth1=0.8 and Cth2=0 as for the TLS model for comparison purposes.

Table 1: Material parameters for both PTR and TLS

Elastic component	C_{11}	91538.5 MPa
	C_{12}	39230.8 MPa
	C_{44}	26153.8 MPa
Slip deformation	$H_1.H_2.H_3$	33 MPa, 0.0005,0.285
	Reference slip rate	0.005
	Rate sensitivity component	0.3
Twinning deformation	$H_1.H_2.H_3$	33 MPa, 0.0005,0.285
	Reference twinning rate	0.005
	Rate sensitivity component	0.3

In the TLS model, the number of active deformation systems is very high. To avoid it, we employed another threshold value for the activation of slip deformations in the twined region. If the twined volume fraction doesn't reach the threshold value, we ignore the contribution of the slip deformation in the twined region to the total deformation.

3.2 Results

Fig.2 shows the stress-strain response of both PTR and TLS simulations. According to this result, there is no clear difference between both methods in tension and compression tests for low values of strain. But, for higher values of strain, the difference is more significative, specially for the compression test. Fig.3 shows the total accumulated twined volume fraction obtained from both methods. According to this result, the twined region's evolution is almost the same for both TLS and PTR methods at low strains. In the compression test at high strain, the PTR method's total accumulated twinning volume fraction is clearly higher than the one obtained from the TLS method. Fig. 4 shows the activation ratio of each system. According to this result, the slip deformation in the twined region was activated in the compression test at high strain. This result demonstrates that the slip deformation in the twined region plays an important role if twinning deformation mechanisms occur extensively.

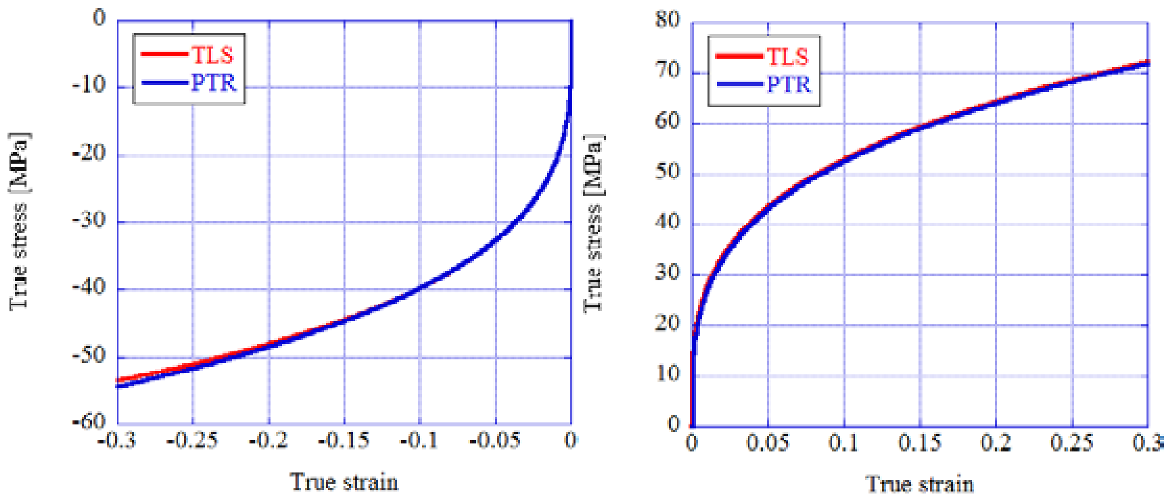

Figure 2: Stress strain reponse of PTR method and TLS

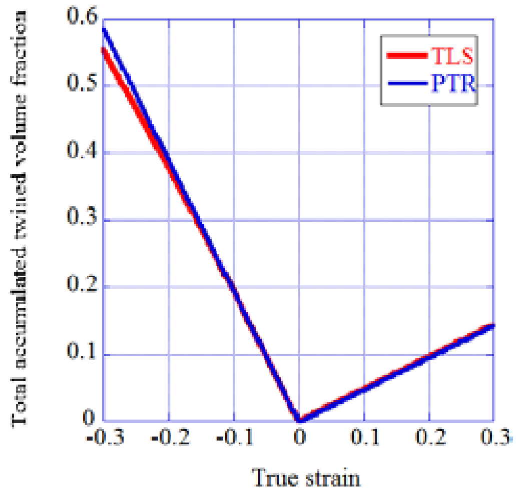

Figure 3: Total accumulated twined volume fraction

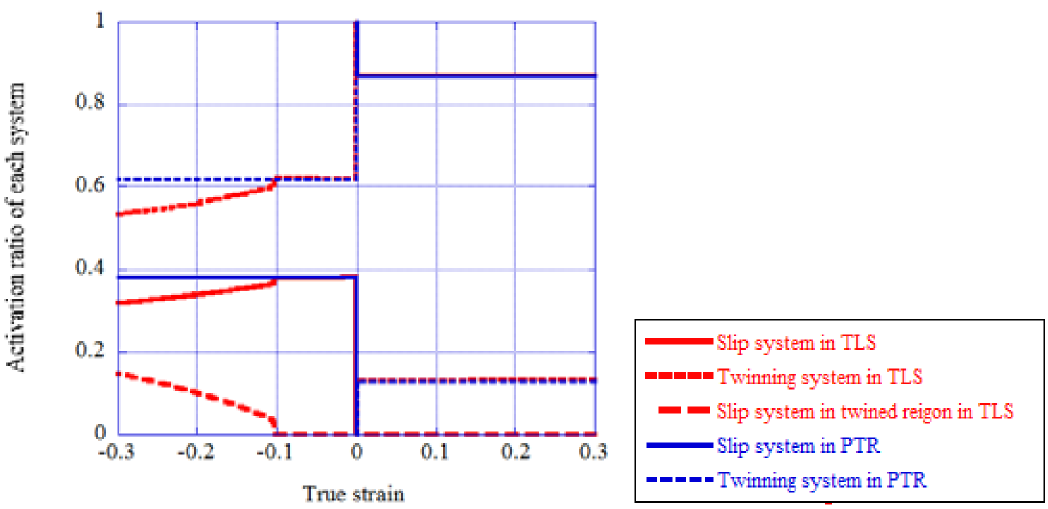

Figure 4: Activation ratio of eash system of PTR method and TLS

4 CONCLUSIONS

- From the crystal plasticity simulations with PTR and TLS twinning models, it can be observed that the TLS compression stress is lower than the one predicted by the PTR model. The main reason for this difference is because the TLS twinning model considers additional slip deformation in the twinned regions.
- The PTR model is simpler, computationally more efficient but less accurate, essentially because of the assumption that twinning mechanism is only active after the twinning volume fraction overcomes a pre-defined threshold value. On the contrary, the TLS model considers twinning effects continuously with more active slip systems, resulting thus in a more accurate prediction for materials with dominant twinning deformation modes.

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